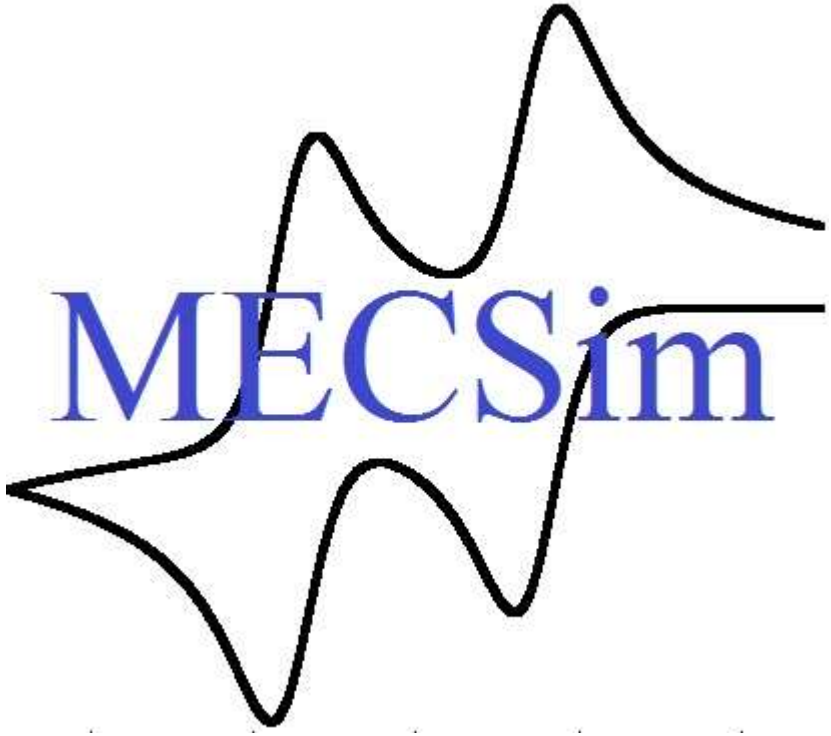
MECSim Summary



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Overview

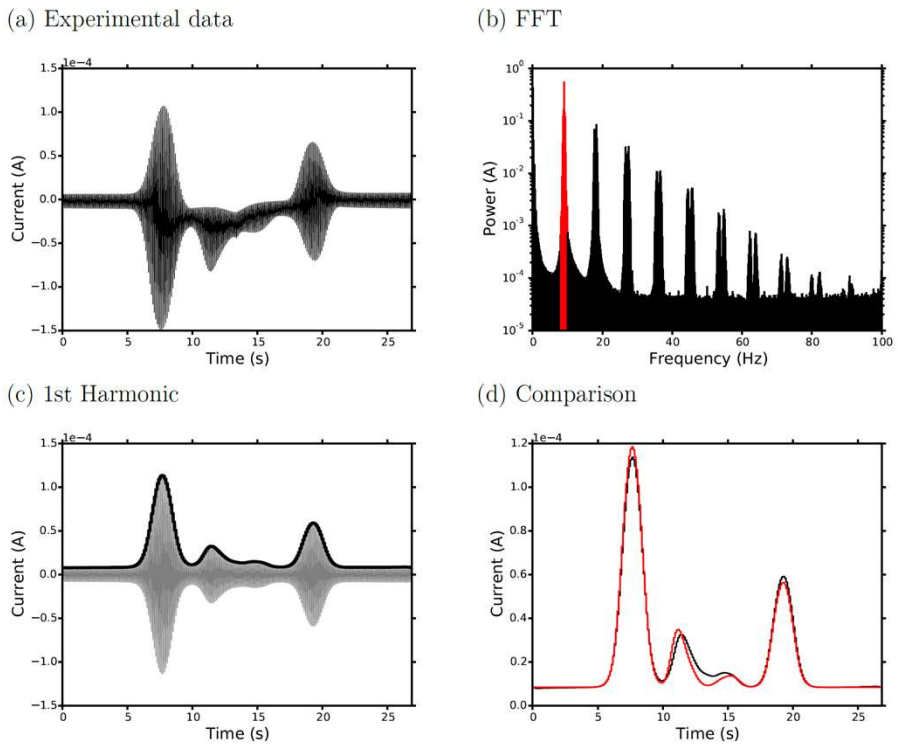
- Brief summary of MECSim
- What is Bayesian inference?
- Error estimation using Bayes
- Introduction to the docker version
  - Video tutorials available here: http://garethkennedy.net/MECSimDocs.html
- Automatic mechanism classifier

Summary of MECSim

- Monash ElectroChemistry Simulator (MECSim)
- Freely downloadable (via Docker for any OS)
- Text file input (Master.inp) and text file output (MECSimOutput_Pot.txt) by design for use on laptop or cluster/cloud
- Can simulate any network of charge transfer and chemical reactions for a range of electrode geometries. Surface confined and solution phase.

Typical simulation output

- Same format as output from potentiostat
- Direct comparison between simulation and experimental data
- Break into harmonics
- Smoothing function
- Comparison via a sum of squares



Bayesian Statistics

Differs from Frequentist interpretation by:

- Fundamentally related to our own certainty or uncertainty of events
- Analyses variation in our believe in different models in terms of fixed observed data
- Can state: given our observed data there is a x% probability that the value of some parameter is within a credible region (often what we want in science)

Bayesian Inference

- Method for updating the ‘belief’ in model
- Bayes’ theorem:

$$P(A \mid B) = \frac{P(B \mid A)\, P(A)}{P(B)}$$

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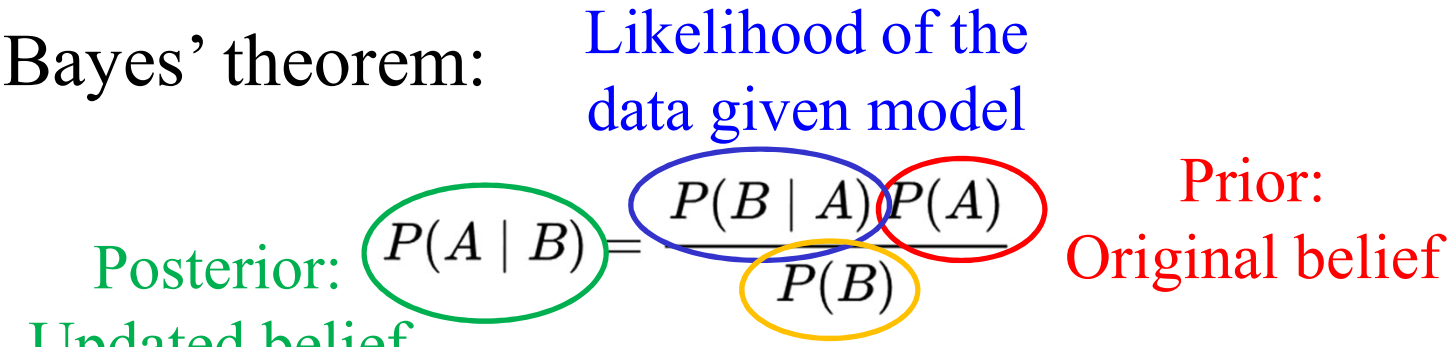

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- Bayes' theorem:

$$P(A \mid B) = \frac{P(B \mid A)\, P(A)}{P(B)}$$

- Bayes' theorem for multiple models M_j given some data x_i

$$P(M_j|\mathbf{x}_i) = \frac{P(M_j)P(\mathbf{x}_i|M_j)}{\sum_{k=1}^{N} P(M_k)P(\mathbf{x}_i|M_k)}$$

Error estimation using Bayes

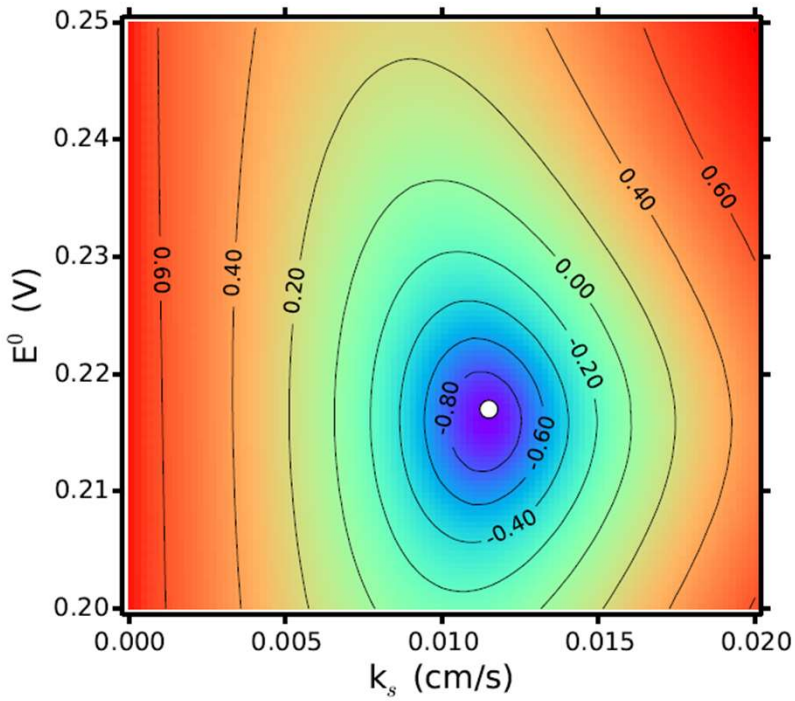
- Have the comparison between the experiment and simulated data from MECSim
- Wish to convert the sum of squares to probability
- Expect relationship: $$P(\mathbf{x}_i|M_j) \sim \frac{1}{E(\mathbf{x}_i|M_j)}$$
- Can estimate then probability by

$$P(\mathbf{x}_i|M_j) = \frac{E_{max}}{E(\mathbf{x}_i|M_j)}$$

$$E(\mathbf{x}_i|M_j) = \chi^2 = \sum_{i=1}^{n}(x_i - f_i(M_j))^2$$

Parameter error estimation

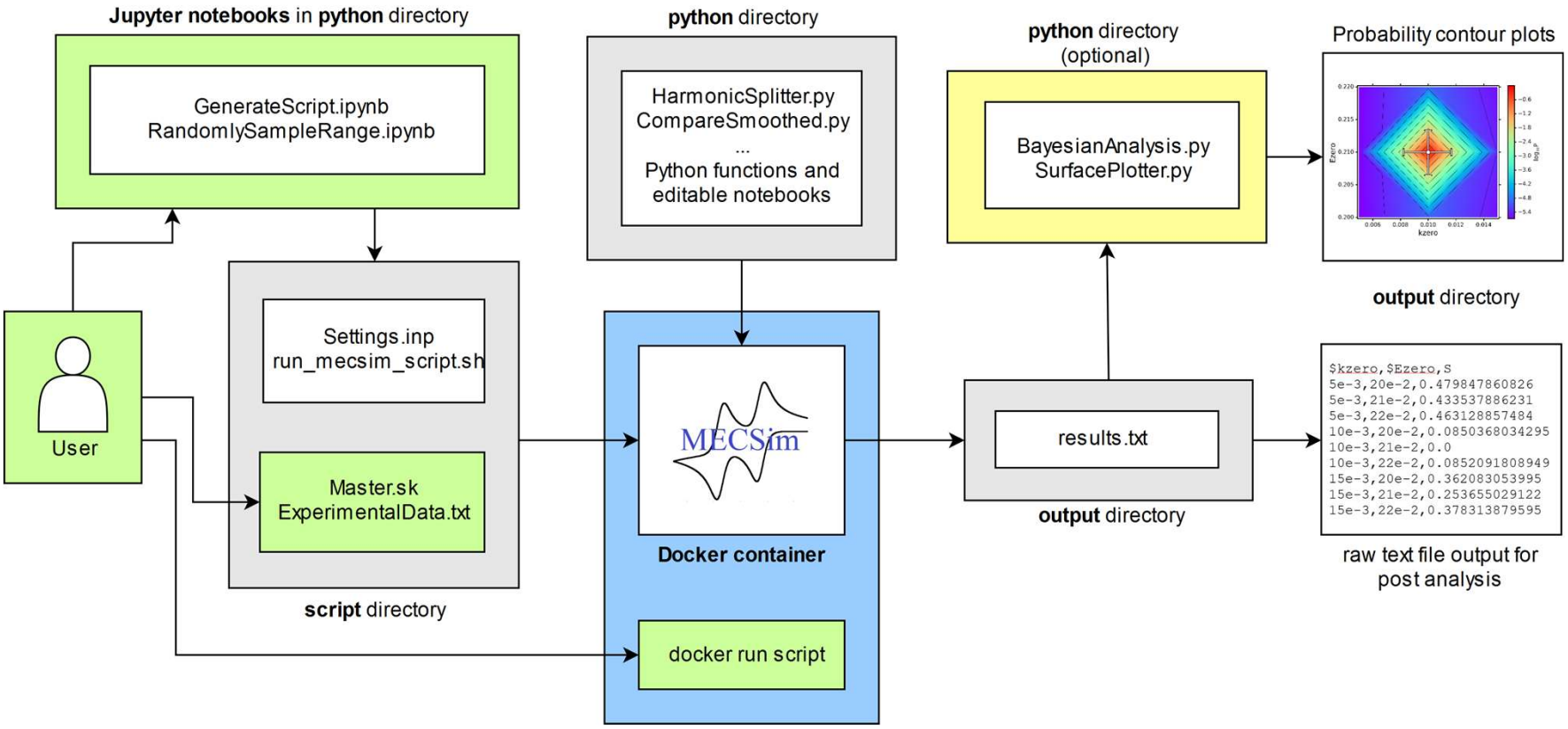
- Combine probabilities for parameter error estimation
- Easier to visualize in 2D but same method applies for N-parameters
- Additional statistical methods can help with N-parameter cases



MECSim docker

- MECSim run internally in a Docker container: allows it to be run on any operating system
- Statistical analysis and parameter sweeps run from Jupyter notebooks using python
- Notebooks are accessible from the docker and your web browser – so no expert computational knowledge required to get started
- Flexible enough so computational experts can add and modify every aspect of it
- Video tutorials now available at: http://garethkennedy.net/MECSimDocs.html

Docker work flow



See live notebook example…